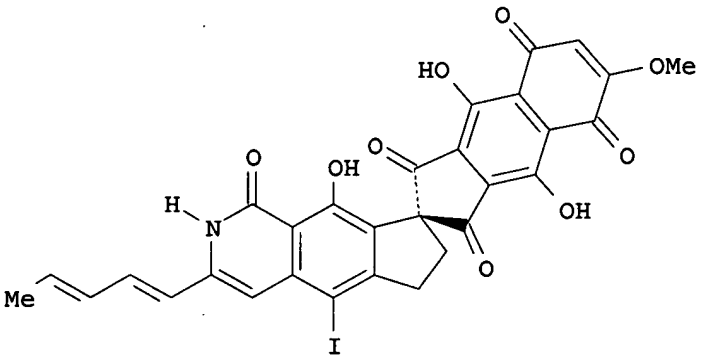
10/511,411

STN- Structure Search 8/15/06

=> d ibib abs hitstr 1-4

L6 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:453919 CAPLUS
DOCUMENT NUMBER: 145:76020
TITLE: Design and semisynthesis of novel fredericamycin A derivatives with an improved antitumor profile
AUTHOR(S): Abel, Ulrich; Simon, Werner; Eckard, Peter; Hansske, Friedrich G.
CORPORATE SOURCE: Santhera Pharmaceuticals, Heidelberg, 69120, Germany
SOURCE: Bioorganic & Medicinal Chemistry Letters (2006), 16(12), 3292-3297
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB The authors report the design, semisynthesis, and biol. activity of a series of fredericamycin derivs. Within this series compound (I) combines low nanomolar cytotoxic potency in vitro, increased tumor cell line selectivity, and in vivo activity in a human xenograft model.

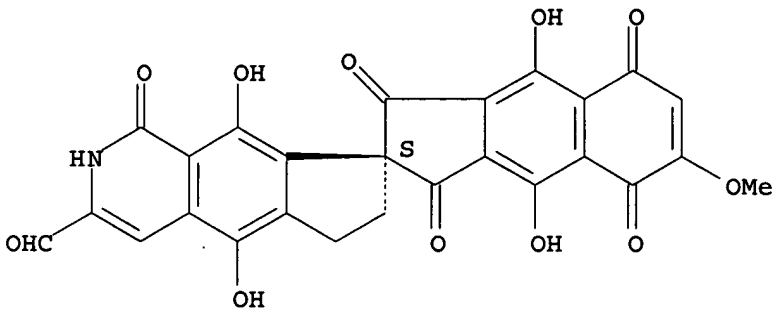
IT 609353-42-6P 609353-48-2P 609353-50-6P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(design and semisynthesis of novel fredericamycin A derivs. with an improved antitumor profile)

RN 609353-42-6 CAPLUS

CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 5'-bromo-6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-(1E,3E)-1,3-pentadienyl-, (2S)- (9CI) (CA INDEX NAME)

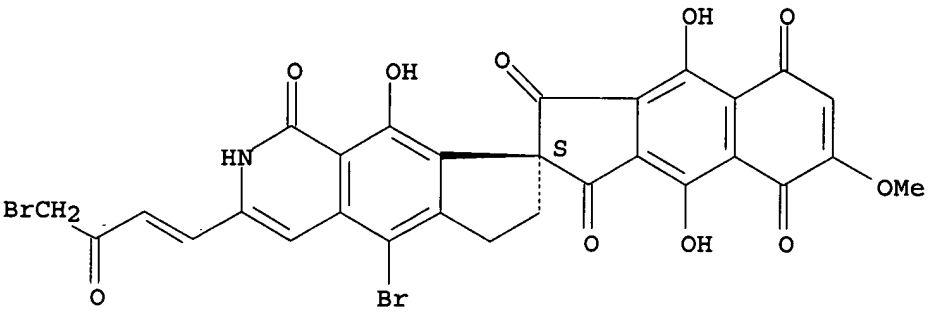
Absolute stereochemistry.
Double bond geometry as shown.

Absolute stereochemistry.



RN 892871-45-3 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8-pentone, 5'-bromo-3'-(4-bromo-3-oxo-1-butenyl)-1',2',6',7'-tetrahydro-4,9,9'-trihydroxy-6-methoxy-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:41264 CAPLUS
DOCUMENT NUMBER: 140:87690
TITLE: Fredericamycin derivatives as medicaments for treating tumors
INVENTOR(S): Simon, Werner; Abel, Ulrich
PATENT ASSIGNEE(S): Biofrontera Pharmaceuticals Holding A.-G., Germany
SOURCE: PCT Int. Appl., 35 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004004713	A1	20040115	WO 2003-EP7427	20030709

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

DE 10230917	A1	20040205	DE 2002-10230917	20020709
CA 2491701	AA	20040115	CA 2003-2491701	20030709
AU 2003250017	A1	20040123	AU 2003-250017	20030709
EP 1519724	A1	20050406	EP 2003-762678	20030709
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2005538069	T2	20051215	JP 2004-518767	20030709
US 2005215579	A1	20050929	US 2005-520421	20050106
PRIORITY APPLN. INFO.:			DE 2002-10230917 A	20020709
			WO 2003-EP7427 W	20030709

OTHER SOURCE(S): MARPAT 140:87690

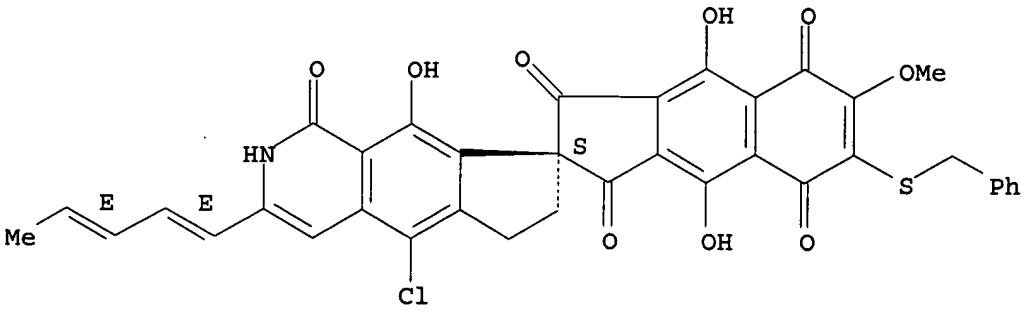
AB The invention discloses fredericamycin derivs., medicaments containing them or their salts, and their use for treating diseases, particularly tumors. Preparation of fredericamycin derivs. is included.

IT 645337-14-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(fredericamycin derivs. as medicaments for treating tumors)

RN 645337-14-0 CAPLUS

CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 5'-chloro-4,9,9'-trihydroxy-6-methoxy-3'-(1E,3E)-1,3-pentadienyl-7-[(phenylmethyl)thio]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:837048 CAPLUS
DOCUMENT NUMBER: 139:337825
TITLE: Preparation of fredericamycin derivatives for use in treating tumors
INVENTOR(S): Werner, Simon; Ulrich, Abel
PATENT ASSIGNEE(S): Bioleads G.m.b.H., Germany
SOURCE: PCT Int. Appl., 45 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 2003087060 A1 20031023 WO 2003-EP3285 20030328
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
DE 10217046 A1 20031106 DE 2002-10217046 20020417
CA 2482775 AA 20031023 CA 2003-2482775 20030328
AU 2003222785 A1 20031027 AU 2003-222785 20030328
EP 1495003 A1 20050112 EP 2003-718715 20030328
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
US 2005153997 A1 20050714 US 2003-511411 20030328
JP 2005528396 T2 20050922 JP 2003-584016 20030328
PRIORITY APPLN. INFO.: DE 2002-10217046 A 20020417
WO 2003-EP3285 W 20030328
OTHER SOURCE(S): CASREACT 139:337825; MARPAT 139:337825
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

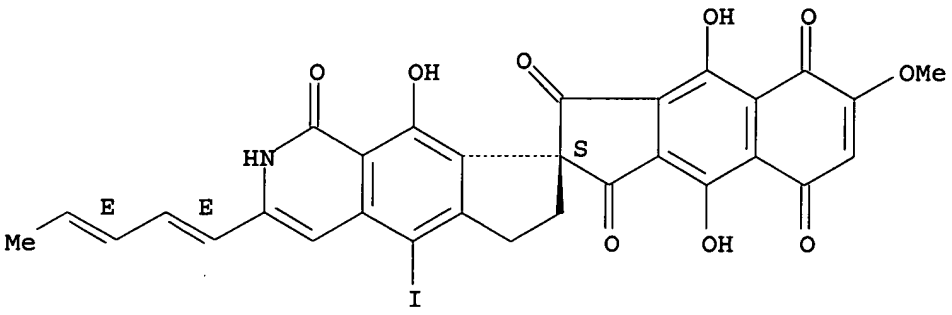
AB The invention relates to novel fredericamycin derivs., e.g., I [R1 = H, C1-6-alkyl, cycloalkyl, (C1-4-alkyl)cycloalkyl; R2 = C1-14-alkyl, C2-14-alkenyl, 1,3-butadienyl, Bu, (C1-4-alkyl)aryl, heteroaryl, (C1-4-alkyl)heteroaryl, cycloalkyl, (C1-4-alkyl)cycloalkyl, heterocycloalkyl, (C1-4-alkyl)heterocycloalkyl, etc.; R3 = C2-14-alkyl, C2-14-alkenyl, C2-14-alkynyl, (un)substiututed aryl, (C1-4-alkyl)aryl, heteroaryl, (C1-4-alkyl)heteroaryl; R4, R6, R7 = H, C1-6-alkyl, COR41; R5 = H, C1-6-alkyl, cycloalkyl, (C1-4-alkyl)cycloalkyl, heterocycloalkyl, (C1-4-alkyl)heterocycloalkyl, aryl, (C1-4-alkyl)aryl, heteroaryl, (C1-4-alkyl)heteroaryl; R41 = C1-14-alkyl, C1-14-alkanoyl, (C1-6-alkyl)oxy, (C1-6-alkyl)amino, (C1-6-alkyl)amino(C1-6-alkyl), (C1-6-alkyl)aminodi(C1-6-alkyl), cycloalkyl, (C1-4-alkyl)cycloalkyl, heterocycloalkyl, (C1-4-alkyl)heterocycloalkyl, aryl, aryloyl, etc.; X = O, S, NH, NR8; R8 = R5; NR5R8 = 4-8 membered heterocyclkoalkyl (with an optional addnl. N, O, S); XR5 = H; Y = O, S, NR9; R9 = H, C1-6-alkyl] and II, or their stereoisomers, tautomers or pharmaceutically acceptable salts, to medicaments containing these derivs., and to the use of them for treating diseases, particularly tumor diseases (no data). Thus, 5-(fluorophenyl)fredericamycin A [III; R2 = CH:CHCH:CHMe-(E,E)] was prepared from fredericamycin A [IV; R2 = CH:CHCH:CHMe-(E,E)] via regioselective iodination with N-iodosuccinimide in DMF followed by arylation with 4-FC6H4B(OH)2 in DMF containing Tl2CO3 and catalytic Pd(Ph3P)4.

IT 609353-43-7P, 5-Iodofredericamycin A
RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation and palladium-catalyzed coupling of, with boronic acids; preparation
of fredericamycin derivs. for use in treating tumors)

RN 609353-43-7 CAPLUS

CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-5'-iodo-6-methoxy-3'-(1E,3E)-1,3-pentadienyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

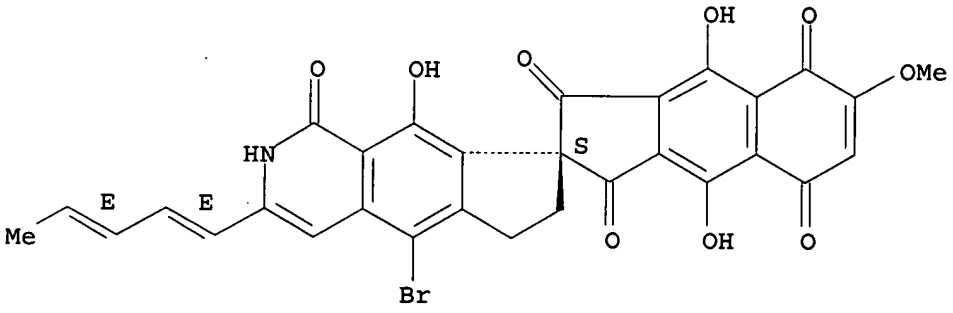


IT 609353-42-6P, 5-Bromofredericamycin A 609353-50-6P, 5-Bromofredericamycin-3-carboxaldehyde 609353-51-7P, 5-Iodofredericamycin-3-carboxaldehyde 616884-46-9P, 5-[(E)-1-Hexenyl]fredericamycin A
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of fredericamycin derivs. for use in treating tumors)

RN 609353-42-6 CAPLUS

CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 5'-bromo-6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-(1E,3E)-1,3-pentadienyl-, (2S)- (9CI) (CA INDEX NAME)

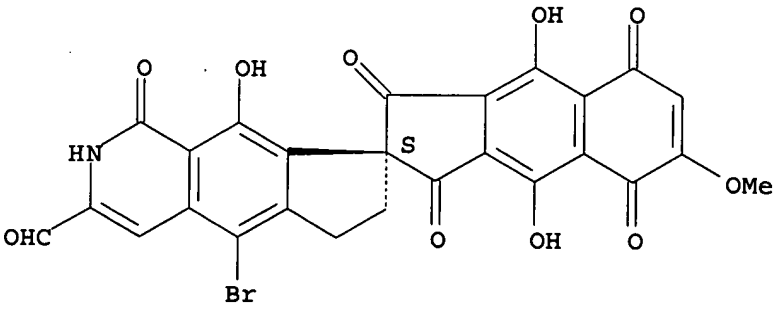
Absolute stereochemistry.
Double bond geometry as shown.



RN 609353-50-6 CAPLUS

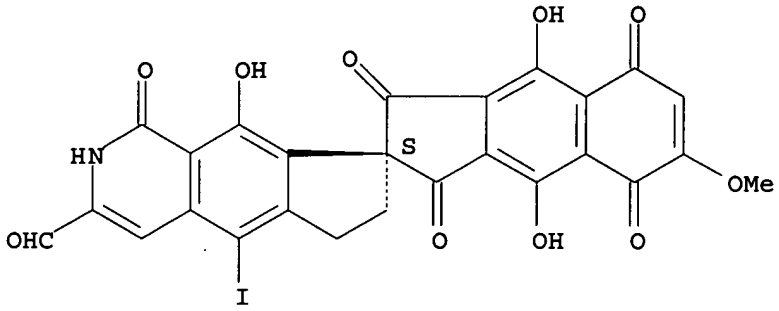
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-3'-carboxaldehyde, 5'-bromo-1,1',2',3,5,6',7',8-octahydro-4,9,9'-trihydroxy-6-methoxy-1,1',3,5,8-pentaoxo-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



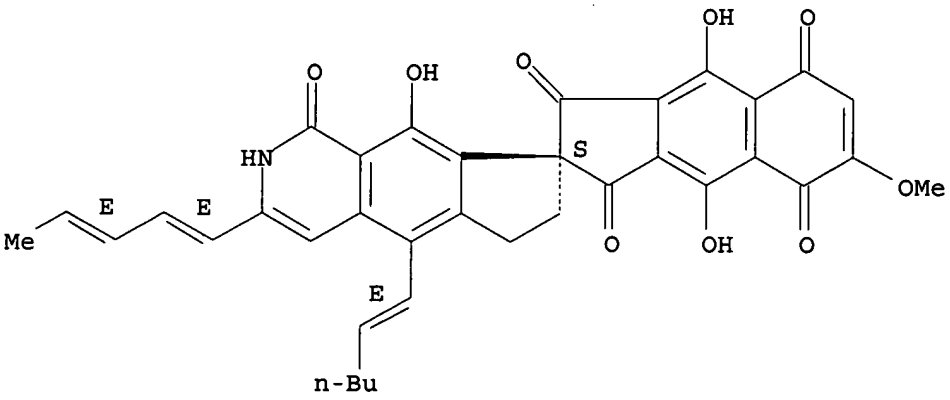
RN 609353-51-7 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-3'-carboxaldehyde, 1,1',2',3,5,6',7',8-octahydro-4,9,9'-trihydroxy-5'-iodo-6-methoxy-1,1',3,5,8-pentaoxo-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 616884-46-9 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 5'-(1E)-1-hexenyl-6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-(1E,3E)-1,3-pentadienyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:777766 CAPLUS
DOCUMENT NUMBER: 139:292095
TITLE: Preparation of fredericamycin derivatives for use in treating cancer
INVENTOR(S): Abel, Ulrich; Simon, Werner
PATENT ASSIGNEE(S): Bioleads GmbH, Germany; Biofrontera Discovery GmbH
SOURCE: PCT Int. Appl., 116 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 2003080582	A2	20031002	WO 2003-EP2922	20030320
WO 2003080582	A3	20041209		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10248451	A1	20031009	DE 2002-10248451	20021017
CA 2480468	AA	20031002	CA 2003-2480468	20030320
AU 2003219088	A1	20031008	AU 2003-219088	20030320
EP 1503988	A2	20050209	EP 2003-714862	20030320
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2005527541	T2	20050915	JP 2003-578337	20030320
US 2005256066	A1	20051117	US 2004-509066	20040924
PRIORITY APPLN. INFO.:			DE 2002-10213580 A	20020326
			DE 2002-10248451 A	20021017
			WO 2003-EP2922 W	20030320

OTHER SOURCE(S): MARPAT 139:292095

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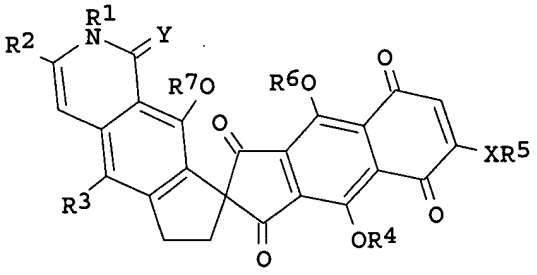

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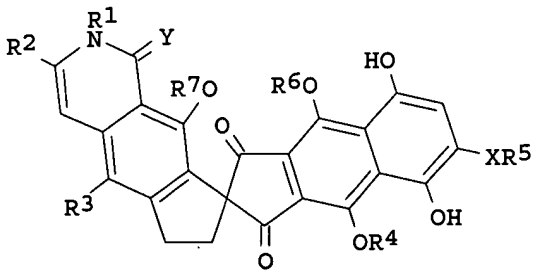
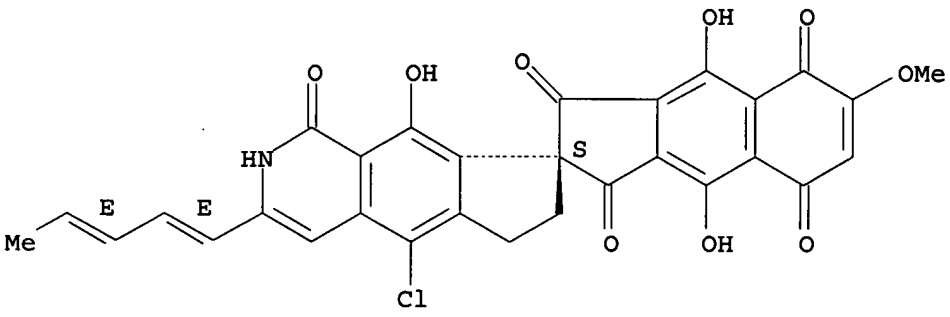


II

AB The invention relates to novel fredericamycin derivs. I [R1 = H, C1-6-alkyl, cycloalkyl, (C1-4-alkyl)cycloalkyl; R2 = H, C1-14-alkyl, C2-14-alkenyl, aryl, (C1-4-alkyl)aryl, heteroaryl, (C1-4-alkyl)heteroaryl, (C2-4-alkenyl)heteroaryl, cycloalkyl, (C1-4-alkyl)cycloalkyl, heterocycloalkyl, (C1-4-alkyl)heterocycloalkyl; R3 = H, F, Cl, Br, I, OH, OR31, NO2, NH2, NHR31, NR31R32, NHCHO, NHCOR31, NHCOCF3, OC(:O)R31; R4,

IT 609353-48-2P, 5-Chlorofredericamycin
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation, osmylation and antitumor activity of; preparation of fredericamycin
derivs. for use in treating cancer)
RN 609353-48-2 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 5'-chloro-6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-(1E,3E)-1,3-pentadienyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



=> d his

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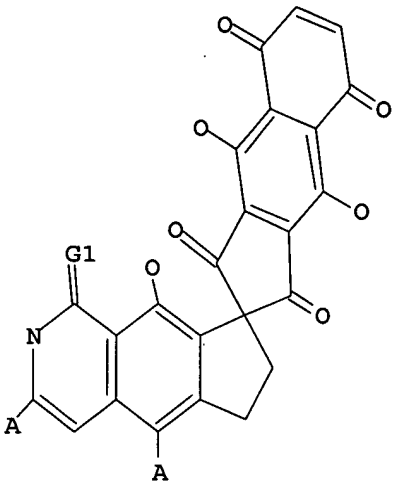
L1 STRUCTURE UPLOADED
L2 13 S L1
L3 STRUCTURE UPLOADED
L4 7 S L3
L5 134 S L3 FULL

FILE 'CAPLUS' ENTERED AT 11:34:16 ON 15 AUG 2006
L6 4 S L5

=> d l3
L3 HAS NO ANSWERS
L3 STR



G1 O,S,N

Structure attributes must be viewed using STN Express query preparation.

=> => d his

(FILE 'HOME' ENTERED AT 11:30:31 ON 15 AUG 2006)

FILE 'REGISTRY' ENTERED AT 11:30:48 ON 15 AUG 2006
L1 STRUCTURE UPLOADED
L2 13 S L1
L3 STRUCTURE UPLOADED
L4 7 S L3
L5 134 S L3 FULL

FILE 'CAPLUS' ENTERED AT 11:34:16 ON 15 AUG 2006
L6 4 S L5

FILE 'REGISTRY' ENTERED AT 11:35:13 ON 15 AUG 2006
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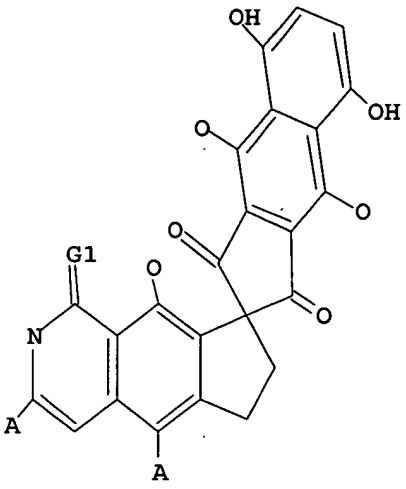
L8 0 S L7
L9 0 S L7 FULL

=> d l7
L7 HAS NO ANSWERS
L7 STR



G1 O,S,N

Structure attributes must be viewed using STN Express query preparation.

=>